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14. ABSTRACT
In this project we have developed reduced basis approximations and associated a posteriori error bounds for parametrized partial differential equations. For this development to be of relevance to AFOSR applications, careful attention has to be paid to numerical analysis; computational procedures; performance assessment; and the application to non-trivial test cases. The approach is at present relevant to linear coercive and noncoercive and nonlinear elliptic equations, linear coercive and weakly noncoercive and nonlinear parabolic equations, and certain classes of linear hyperbolic equations. Applications considered include heat transfer, acoustics, elasticity, fluid dynamics, and electromagnetics.

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REDUCED BASIS APPROXIMATION AND *A POSTERIORI* ERROR ESTIMATION FOR PARAMETRIZED PARTIAL DIFFERENTIAL EQUATIONS

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Abstract

In this project we have developed reduced basis approximations and associated a posteriori error bounds for parametrized partial differential equations. For this development to be of relevance to AFOSR applications, careful attention has to be paid to numerical analysis; computational procedures; performance assessment; and the application to non-trivial test cases. The approach is at present relevant to linear coercive and noncoercive and nonlinear elliptic equations, linear coercive and weakly noncoercive and nonlinear parabolic equations, and certain classes of linear hyperbolic equations. Applications considered include heat transfer, acoustics, elasticity, fluid dynamics, and electromagnetics.

We describe below the many methodological advances completed during the course of this grant. In all cases the emphasis is on fast response in the real-time or many-query context certified by rigorous *a posteriori* error estimators with the application to complex non-trivial test cases.

Overview of Contributions and Core Efforts

Note: Numbers in parenthesis refer to papers listed below.

Improved Inf-Sup Calculation and Successive constraint methods [4,5,8].
In the area of frequency-domain wave phenomena — relevant to acoustics, elastodynamics, and electromagnetics — we have significantly improved the Offline-Online calculation of the inf-sup stability factor crucial to our rigorous error bounds. The new approach combines attractive features of earlier "natural norm" and "Successive Constraint Method" techniques to achieve a demonstrated order of magnitude improvement in performance in particular in the Offline stage of the calculation. This has also significantly improved the accuracy and speed of the error estimator, in particular for problems with resonant or near-resonant behavior. Examples are presented for acoustics and electromagnetics.

Certified Reduced Basis Methods for Maxwell's Equations [10,17].
We have developed certified reduced basis methods for the efficient and reliable evaluation of a

general output that is implicitly connected to a given parameterized input through the harmonic Maxwell's equations. The truth approximation and the development of the reduced basis through a greedy approach is based on a discontinuous Galerkin approximation. The formulation and analysis is very general and allows the use of different approximation spaces for solving the primal and the dual truth approximation problems to respect the characteristics of both problem types. The main features of the method are: *i*) rapid convergence on the entire set of parameters, *ii*) rigorous a posteriori error estimators for the output and *iii*) off-line/on-line phases to enable the rapid solution of many query problems arising in control, optimization, and design. The versatility and performance of this approach has been demonstrated both for highly complex internal problems with multiple resonances and external problems with scattering applications. Speedup of the the reduced basis method when compared to the truth approximation is as much as two orders of magnitude.

For scattering applications we have also demonstrated the ability to parameterize both geometries and frequencies with excellent results and speedups comparable to those discussed above.

Empirical Interpolation Method: Rigorous Error Bounds and Improved Performance [9, 17]
For problems non-affine in the parameter the Empirical Interpolation Method offers an effective approach for reduction to approximation affine form — a prerequisite for subsequent effective Offline-Online strategies. However, until recently, no rigorous error bounds were available to quantify the Empirical Interpolation Method error. In this grant we have developed rigorous error bounds which can (*i*) provide complete certification which includes both reduced basis and empirical interpolation errors, and (*ii*) permit efficient Empirical Interpolation Method truncation.

Furthermore for complex non-affine functions such as those appearing in integral equation kernels, the empirical interpolation methods leads to long expansions to secure adequate accuracy. This directly impacts the online evaluation cost. We have developed a hierarchical improvement which, in a greedy fashion, builds the empirical interpolation approach. A simple online search and a rapid evaluation then allows the online evaluation of the output of interest. This has dramatically accelerate problems where long interpolations are needed and have, in particular, proven to be essential for the development of fast and efficient reduced basis methods for problems formulated on integral form.

Unsteady Incompressible Fluid Flows [3,7].
In the area of nonlinear parabolic equations and in particular unsteady incompressible fluid flows we have extended our certified reduced basis approach to the Burgers equation and to the Navier-Stokes Boussinesq equations of natural convection (relevant, for example, to materials processing) . The certified error bounds restrict the domain of application to modest times (order the diffusive timescale, or many convective timescales) and also modest Reynolds/Grashof. However, within this envelope, the reduced basis method (in the Online stage) is very efficient relative to classical approaches.

h-p Approaches [13,16]
We have developed new *h-p* reduced basis approaches for elliptic and parabolic equations. In these approaches we first optimally divide the parameter domain into subdomains ("*h*-type" refinement); we then pursue the standard "*p*-type" reduced basis refinement in each subdomain. The *h-p* approach is crucial in preserving low Online cost in particular for larger parameter domains. The method is particularly well-suited to quadratically nonlinear problems (such as Navier-Stokes).

Parallel Approaches [18].
The Offline stage of the reduced basis method is expensive, in particular for three-dimensional spatial domains and large parameter domains. We have developed new parallel procedures that exploit concurrency in both the spatial domain and the parameter domain. Implementation and tests were performed on the Ranger supercomputer at TACC.

Hierarchical Architectures [14,18].
The Online stage of the reduced basis method is very inexpensive — requires little memory and little processing power. This suggests implementation of the Offline stage on a supercomputer (see above) and implementation of the Online stage on slim platforms — to facilitate real-time many-query calculations "in the field" (e.g., parameter estimation, embedded control). We have demonstrated this concept with an implementation of the Online stage on a Nexus One Smartphone.

Multiscale Analysis [6, 15].
In the area of multiscale analysis — reduced basis techniques for rapid repeated evaluation of microscale-induced effective properties — we have extended earlier work in the homogenization context to the more challenging area of complex flows (relevant, for example, to polymer- or biomolecule-laden fluids) governed by coupled Stokes Fokker-Planck systems.

Uncertainty Quantification [2, 12].
In the area of uncertainty analysis, we have incorporated our reduced basis approximations and associated error bounds into both Bayesian parameter estimation frameworks and stochastic partial differential equation frameworks: the approach yields rigorous assessments of both numerical and parametric model errors in (currently) thermal systems.

Reduced Basis Methods for Integral Equations[17]
We have begun the development of an reduced basis method as an efficient tool for parametrized scattering problems in computational electromagnetics in cases where field solutions are computed using a standard Boundary Element Method (BEM) for the parametrized Electric Field Integral Equation (EFIE). The significant complicate here as compared to all previous work is the highly non-affine nature of the kernels and sources, requiring use to develop robust and accurate ways of dealing with this through empirical interpolation. The problems are parameterized by the wavenumber, the angle of the incident plane wave and its polarization, hence enabling a rapid evaluation of scattering and scattering signatures for problems in which the truth approximation is an integral equation solver as is often the case in complex applications. As for differential equation truth approximations, the potential for speedup is considerable and exceeds 10 for even simple applications such a spheres and cavities.

Reduced Basis Element Methods for Electromagnetics[11]
We have demonstrated a reduced basis element method (RBEM) for the time-harmonic Maxwells equation. The RBEM is a Reduced Basis Method (RBM) with parameters describing the geometry of the computational domain, coupled with a domain decomposition method. The basic idea is to first decompose the computational domain into a series of subdomains, each of which is deformed from some reference domain, and then to associate with each reference domain precomputed solutions to the same governing partial differential equation, but with different choices of deformations. Finally one seeks the approximation on a new shape as a linear combination of the corresponding precomputed solutions on each subdomain. Unlike the work on RBEM for thermal fin and fluid

flow problems, we do not need a mortar type method to glue the various local functions. This gluing is done automatically thanks to the use of a discontinuous Galerkin method. We introduced the methods and presented numerical results showing exponential convergence for the simulation of a metallic pipe with both ends open. We have also developed some theoretical understanding of the a posteriori error estimate for RBEM.

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Honors & Awards received

The Springer Computational Science and Engineering Prize 2009 (for research teams of young investigators) was awarded to DBP Huynh, NC Nguyen, and G Rozza for development of the certified reduced basis software package rbMIT © MIT. Huynh, Nguyen, and Rozza are all former Singapore-MIT Alliance or MIT students or postdoctoral associates (supervised by Patera and) supported by the Singapore-MIT Alliance and AFOSR Grants FA9550-05-1-0114 or FA9550-07-1-0425.

Technology Transfer

Throughout the project there has been a close contact to HyperComp Inc (Los Angeles, CA) who continues to pursue the development of certified reduced basis methods as part of their in-house modeling software, used extensively for solving classified and high complex AFRL applications. The ongoing development demonstrated in this effort has allowed them to seek the development of a high-quality reduced basis technique with particular applications to scattering applications.

Much of the (linear) RB technology that we have developed is available in a software package rbMIT which can be downloaded from our website `http://augustine.mit.edu/methodology/methodology_rbMIT_System.htm` (subject to usual academic license restrictions).

We have developed a high-performance implementation of the certified reduced basis method, rbOOmit, based on the C++ finite element library libMesh. This code is available under an open source license as part of the libMesh project. See `http://libmesh.sourceforge.net` for more details.

We also developed a reduced basis front-end, rbAPPmit, that runs on Android smartphones. This "app" is available for download from the website `http://sourceforge.net/projects/rbappmit/`.